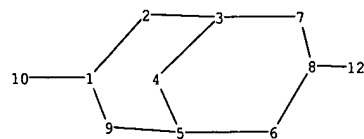
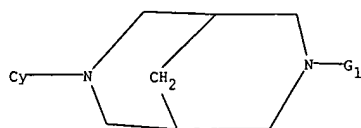


Search after amendment  
No prior art. → found.



chain nodes :

10 12

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

1-10 8-12

ring bonds :

1-2 1-9 2-3 3-4 3-7 4-5 5-6 5-9 6-8 7-8

exact/norm bonds :

1-2 1-9 1-10 2-3 3-4 3-7 4-5 5-6 5-9 6-8 7-8 8-12

G1:H,CH3,Et,n-Pr,i-Pr,n-Bu

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS

Generic attributes :

10:

Saturation : Unsaturated

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspal611hxl

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Apr 08	"Ask CAS" for self-help around the clock
NEWS	3	Jun 03	New e-mail delivery for search results now available
NEWS	4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS	5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS	6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS	7	Sep 03	JAPIO has been reloaded and enhanced
NEWS	8	Sep 16	Experimental properties added to the REGISTRY file
NEWS	9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS	10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS	11	Oct 24	BEILSTEIN adds new search fields
NEWS	12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS	13	Nov 18	DKILIT has been renamed APOLLIT
NEWS	14	Nov 25	More calculated properties added to REGISTRY
NEWS	15	Dec 04	CSA files on STN
NEWS	16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS	17	Dec 17	TOXCENTER enhanced with additional content
NEWS	18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS	19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS	20	Feb 13	CANCERLIT is no longer being updated
NEWS	21	Feb 24	METADEX enhancements
NEWS	22	Feb 24	PCTGEN now available on STN
NEWS	23	Feb 24	TEMA now available on STN
NEWS	24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS	25	Feb 26	PCTFULL now contains images
NEWS	26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS	27	Mar 19	APOLLIT offering free connect time in April 2003
NEWS	28	Mar 20	EVENTLINE will be removed from STN
NEWS	29	Mar 24	PATDPAFULL now available on STN
NEWS	30	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS	31	Apr 11	Display formats in DGENE enhanced
NEWS	32	Apr 14	MEDLINE Reload
NEWS	33	Apr 17	Polymer searching in REGISTRY enhanced
NEWS	34	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS	35	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS	36	Apr 28	RDISCLOSURE now available on STN
NEWS	37	May 05	Pharmacokinetic information and systematic chemical names added to PHAR

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT

05/14/2003

09864905.trn

MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:06:36 ON 14 MAY 2003

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:06:44 ON 14 MAY 2003  
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 MAY 2003 HIGHEST RN 514787-08-7  
DICTIONARY FILE UPDATES: 13 MAY 2003 HIGHEST RN 514787-08-7

TSKA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

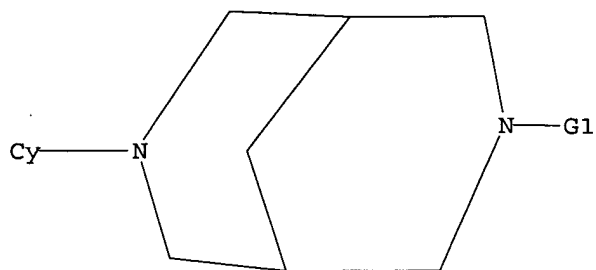
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 09864905.str

L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



G1 H, Me, Et, n-Pr, i-Pr, n-Bu

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:07:01 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 10182 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

1 ANSWERS

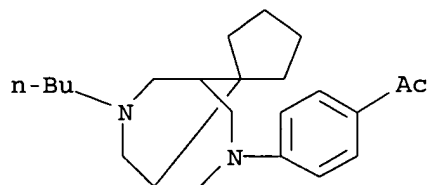
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 197599 TO 209681  
PROJECTED ANSWERS: 12 TO 394

L2 1 SEA SSS SAM L1

=> d scan

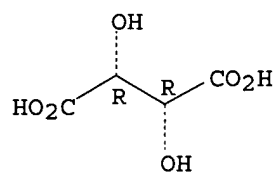
L2 1 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Ethanone, 1-[4-(7'-butylspiro[cyclopentane-1,9'-  
[3,7]diazabicyclo[3.3.1]nonan]-3'-yl)phenyl]-, (2R,3R)-2,3-  
dihydroxybutanedioate (1:1) (9CI)  
MF C23 H34 N2 O . C4 H6 O6

CM 1



CM 2

Absolute stereochemistry.



ALL ANSWERS HAVE BEEN SCANNED

05/14/2003

09864905.trn

=>

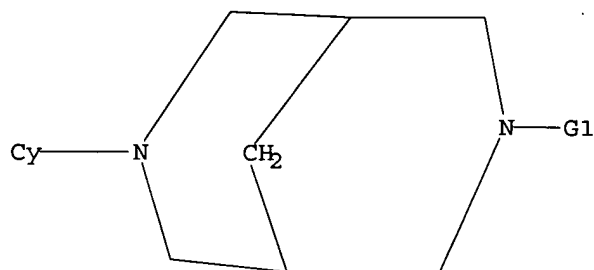
Uploading 09864905.str

L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS

L3 STR



G1 H, Me, Et, n-Pr, i-Pr, n-Bu

Structure attributes must be viewed using STN Express query preparation.

=> s l3

SAMPLE SEARCH INITIATED 11:15:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 10182 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 197599 TO 209681  
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> s l3 ful

FULL SEARCH INITIATED 11:15:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 205488 TO ITERATE

100.0% PROCESSED 205488 ITERATIONS 40 ANSWERS  
SEARCH TIME: 00.00.05

L5 40 SEA SSS FUL L3

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	153.35	153.56

FILE 'CAPLUS' ENTERED AT 11:15:24 ON 14 MAY 2003

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FILE COVERS 1907 - 14 May 2003 VOL 138 ISS 20  
FILE LAST UPDATED: 13 May 2003 (20030513/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

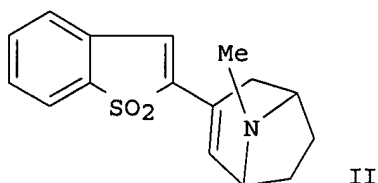
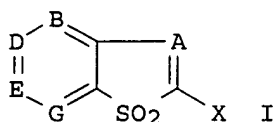
L6                    5 L5

=> d abs ibib hitstr 1-

YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

~~86~~  
 GI

ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS



AB Novel compds. of formula I [A, B, D, E, G = C, N; X = heterocycle] are prepd. that are found to be cholinergic ligands at the nicotinic acetylcholine receptors and modulators of the monoamine receptors and transporters. Due to their pharmacol. profile the compds. of the invention may be useful for the treatment of diseases or disorders as diverse as those related to the cholinergic system of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances. Thus, was prepd. and inhibited 3H-.alpha.-bungarotoxine binding in rat brain with IC50 of 0.018 .mu.M.

ACCESSION NUMBER: 2003:42270 CAPLUS

DOCUMENT NUMBER: 138:89958

TITLE: Preparation of benzothiophene and benzothiazole compounds as cholinergic and monoamine receptor modulators

INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet  
Ostergaard; Ahring, Philip K.; Jorgensen, Tino Dyhring

PATENT ASSIGNEE(S): Neurosearch A/S, Den.

SOURCE: PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003004493	A1	20030116	WO 2002-DK460	20020702
WO 2003004493	C1	20030410		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: DK 2001-1064 A 20010706

OTHER SOURCE(S): MARPAT 138:89958

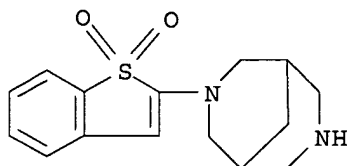
IT 484651-51-6P 484651-52-7P 484651-59-4P  
484651-60-7P



RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of benzothiophene and benzothiazole compds. as cholinergic and monoamine receptor modulators)

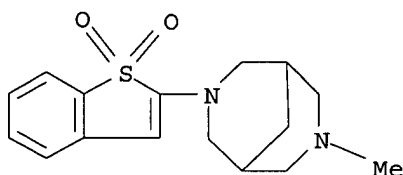
RN 484651-51-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1,1-dioxidobenzo[b]thien-2-yl) - (9CI)  
(CA INDEX NAME)



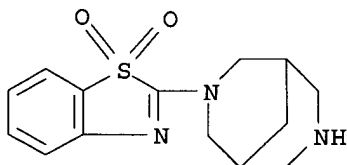
RN 484651-52-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1,1-dioxidobenzo[b]thien-2-yl)-7-methyl- (9CI) (CA INDEX NAME)



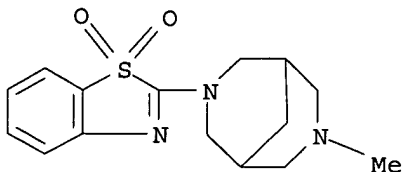
RN 484651-59-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1,1-dioxido-2-benzothiazolyl) - (9CI)  
(CA INDEX NAME)



RN 484651-60-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1,1-dioxido-2-benzothiazolyl)-7-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

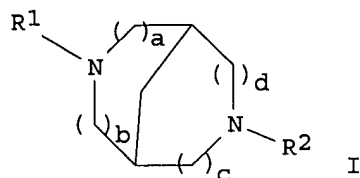
8

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

05/14/2003

09864905.trn

~~L6~~ ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS  
GI



AB The present invention relates to novel diazabicycloalkanes (shown as I; a/b/c/d = 1,1,1,1, 1,1,1,2, 1,1,2,1, 0,2,0,2 and 0,0,2,2; see below for addnl. definitions of variables; e.g. 3-benzyl-7-(6-phenyl-3-pyridazinyl)-3,7-diazabicyclo[3.3.1]nonane), their labeled or unlabeled forms, any of their enantiomers, any mixt. of enantiomers, or pharmaceutically acceptable salts thereof or a prodrug thereof, which are cholinergic ligands at the nicotinic acetylcholine receptors and modulators of the monoamine receptors and transporters. Due to their pharmacol. profile the compds. of the invention may be useful for the treatment of diseases or disorders as diverse as those related to the cholinergic system of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances. A diazabicycloalkane deriv. = those represented by Formula I, by Formula II, by Formula III, by Formula IV, and by Formula V. For I: n = 1, 2 or 3; R1 = H, alkyl, cycloalkyl, cycloalkylalkyl, alkenyl, alkenylalkyl, alkynyl, alkynylalkyl, aryl, aralkyl or fluorescent group, which aryl groups may be substituted .gtoreq.1 times with substituents alkyl, cycloalkyl, cycloalkylalkyl, alkenyl, alkynyl, methylenedioxy, hydroxy, alkoxy, alkoxyalkyl, alkoxyalkoxy, aryloxy, sulfhydryl, thioalkoxy, alkylcarbonyloxy, halogen, CF3, OCF3, CN, and nitro; and/or which aryl groups may be substituted with .gtoreq.1 fluorescent groups. R2 = a mono- or polycyclic aryl group, or a mono- or poly-heterocyclic group, which aryl and heterocyclic groups may be substituted .gtoreq.1 times with substituents alkyl, cycloalkyl, cycloalkylalkyl, alkenyl, alkynyl, methylenedioxy, hydroxy, alkoxy, alkoxyalkyl, alkoxyalkoxy, aryloxy, sulfhydryl, thioalkoxy, alkylcarbonyloxy, halogen, CF3, OCF3, CN, and nitro; or which heterocyclic group may be substituted once with another mono- or poly-heterocyclic group, a mono- or polycyclic aryl group, or a mono- or polycyclic aralkyl group; and/or which heterocyclic group may be substituted with .gtoreq.1 fluorescent groups. Although the methods of prepn. are not claimed, several example prepn. of I and intermediates are included and about 20 I are listed in the claims. Results for tabulated for two I regarding in vitro inhibition of 3H-5-Hydroxytryptamine (3H-5-HT, serotonin) uptake in cortical synaptosomes (e.g. IC50 = 0.022 .mu.M for 3-benzyl-7-(2-quinolinyl)-3,7-diazabicyclo[3.3.1]nonane) and in vitro inhibition of 3H-cytisine binding (e.g. IC50 = 0.0030 for 7-(6-chloro-3-pyridazinyl)-3,7-diazabicyclo[3.3.1]nonane).

ACCESSION NUMBER: 2002:927433 CAPLUS  
DOCUMENT NUMBER: 138:14081  
TITLE: Preparation of heteroaryl diazabicycloalkanes as central nervous system modulators  
INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet

Ostergaard; Ahring, Philip K.; Jorgensen, Tino  
 Dyhring; Sloek, Frank Abildgaard  
 PATENT ASSIGNEE(S): Neurosearch A/S, Den.  
 SOURCE: PCT Int. Appl., 49 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096911	A1	20021205	WO 2002-DK347	20020523
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PRIORITY APPLN. INFO.: DK 2001-866 A 20010601

OTHER SOURCE(S): MARPAT 138:14081

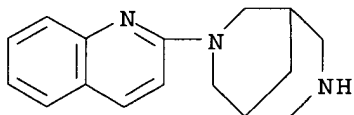
IT 345317-26-2P, 7-(2-Quinoliny)-3,7-diazabicyclo[3.3.1]nonane

477602-85-0P, 7-(6-Phenyl-3-pyridaziny)-3,7-diazabicyclo[3.3.1]nonane

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (drug candidate; prepn. of heteroaryl diazabicycloalkanes as central nervous system modulators)

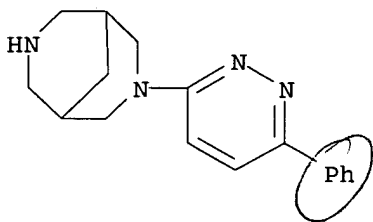
RN 345317-26-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-quinoliny)- (9CI) (CA INDEX NAME)



RN 477602-85-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-phenyl-3-pyridaziny)- (9CI) (CA INDEX NAME)



IT 477602-84-9P, 7-(2-Quinoliny)-3,7-diazabicyclo[3.3.1]nonane  
 fumaric acid salt 477602-86-1P, 7-(6-Phenyl-3-pyridaziny)-3,7-diazabicyclo[3.3.1]nonane fumaric acid salt 477602-98-5P,

3-Methyl-7-(6-phenyl-3-pyridazinyl)-3,7-diazabicyclo[3.3.1]nonane

**477602-99-6P**, 3-Methyl-7-(6-phenyl-3-pyridazinyl)-3,7-diazabicyclo[3.3.1]nonane fumaric acid salt **477603-03-5P**,

7-(6-Chloro-3-pyridazinyl)-3,7-diazabicyclo[3.3.1]nonane

**477603-04-6P**, 7-(6-Chloro-3-pyridazinyl)-3,7-diazabicyclo[3.3.1]nonane fumaric acid salt **477603-05-7P**,

7-(6-Chloro-2-pyrazinyl)-3,7-diazabicyclo[3.3.1]nonane

**477603-06-8P**, 7-(6-Chloro-2-pyrazinyl)-3,7-diazabicyclo[3.3.1]nonane fumaric acid salt **477603-08-0P**,

3-Methyl-7-(2-quinolinyl)-3,7-diazabicyclo[3.3.1]nonane

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of heteroaryl diazabicycloalkanes as central nervous system modulators)

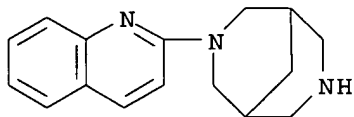
RN 477602-84-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-quinolinyl)-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

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CRN 345317-26-2

CMF C16 H19 N3

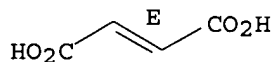


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



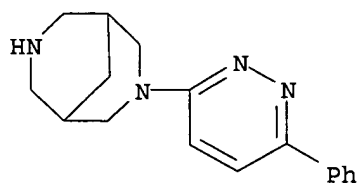
RN 477602-86-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-phenyl-3-pyridazinyl)-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 477602-85-0

CMF C17 H20 N4

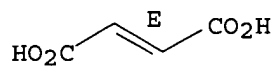


CM 2

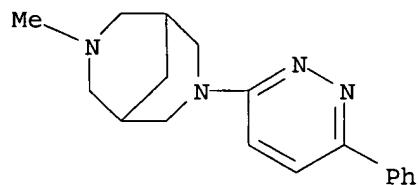
CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 477602-98-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-methyl-7-(6-phenyl-3-pyridazinyl)- (9CI)  
(CA INDEX NAME)

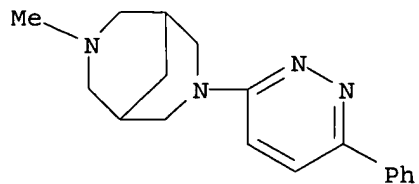
RN 477602-99-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-methyl-7-(6-phenyl-3-pyridazinyl)-,  
(2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 477602-98-5

CMF C18 H22 N4

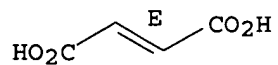


CM 2

CRN 110-17-8

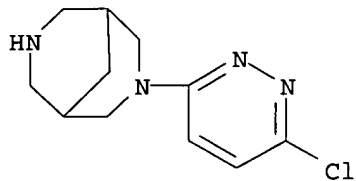
CMF C4 H4 O4

Double bond geometry as shown.



RN 477603-03-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridazinyl)- (9CI) (CA INDEX NAME)



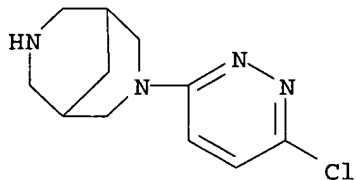
RN 477603-04-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridazinyl)-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 477603-03-5

CMF C11 H15 Cl N4

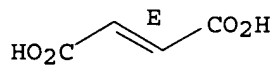


CM 2

CRN 110-17-8

CMF C4 H4 O4

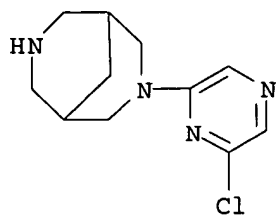
Double bond geometry as shown.



RN 477603-05-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloropyrazinyl)- (9CI) (CA INDEX NAME)

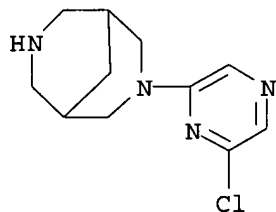
6



RN 477603-06-8 CAPLUS  
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloropyrazinyl)-, (2E)-2-butenedioate  
 (9CI) (CA INDEX NAME)

CM 1

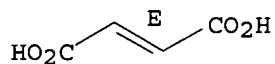
CRN 477603-05-7  
 CMF C11 H15 Cl N4



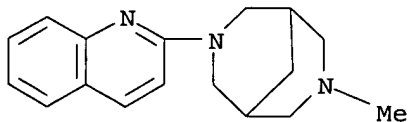
CM 2

CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 477603-08-0 CAPLUS  
 CN 3,7-Diazabicyclo[3.3.1]nonane, 7-methyl-3-(2-quinoliny)- (9CI) (CA INDEX  
 NAME)

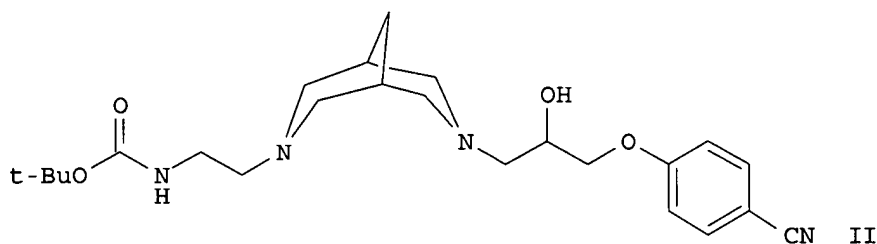
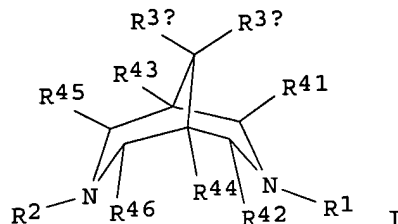


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



16  
GI

ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS



AB The title compds. [I; R1 = ACR4R5BR6 (wherein R4 = H, halo, alkyl, etc.; or R4, together with R5, = O; R5 = H, alkyl,; A = a bond, alkylene, etc.; B = a bond, alkylene, etc.; R6 = (un)substituted aryl, 5-12 membered heterocyclyl contg. one or more heteroatoms selected from O, N and/or S); R2 = CN, (un)substituted 5-12 membered heterocyclyl contg. one or more heteroatoms selected from O, N and/or S, etc.; R3a, R3b = H, alkyl, etc.; or R3a and R3b together = alkylene, O(alkylene)O, etc.; R41-R46 = H, alkyl] which are useful in the prophylaxis and in the treatment of arrhythmias, in particular atrial and ventricular arrhythmias, were prepd. E.g., a 3-step synthesis of II was given. The exemplified compds. I showed pIC50 of at least 5.5 in glucocorticoid-treated mouse fibroblasts as a model to detect blockers of the delayed rectifier K current.

ACCESSION NUMBER: 2002:51458 CAPLUS

DOCUMENT NUMBER: 136:118479

TITLE: Preparation of new bispidine compounds for the treatment of cardiac arrhythmias

INVENTOR(S): Andersson, Kjell; Bjoere, Annika; Bjoersne, Magnus; Ponten, Fritiof; Strandlund, Gert; Svensson, Peder; Tottie, Louise

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

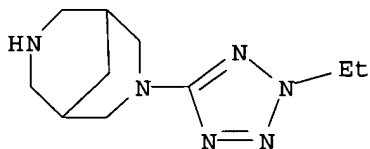
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004446	A1	20020117	WO 2001-SE1544	20010704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

05/14/2003

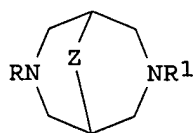
09864905.trn

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,  
 RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,  
 UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 EP 1301510 A1 20030416 EP 2001-950132 20010704  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 NO 2003000057 A 20030131 NO 2003-57 20030106  
 PRIORITY APPLN. INFO.: SE 2000-2603 A 20000707  
 SE 2000-2788 A 20000727  
 WO 2001-SE1544 W 20010704  
 OTHER SOURCE(S): MARPAT 136:118479  
 IT **389887-72-3P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. of new bispidine compds. for the treatment of cardiac  
 arrhythmias)  
 RN 389887-72-3 CAPLUS  
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-ethyl-2H-tetrazol-5-yl)- (9CI) (CA  
 INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS  
GI



I

AB Title compds. [I; Z = (CH<sub>2</sub>)<sub>n</sub>; n = 0-2; R = H, alkyl, aryl, aralkyl, fluorescent group; R<sub>1</sub> = (substituted) mono- or polyheterocyclyl], were prepd. as drugs and diagnostic agents (no data). Thus, 3,7-dibenzyl-3,7-diazabicyclo[3.3.1]nonane (prepn. given) was stirred with HCO<sub>2</sub>H and Pd/C to give crude monobenzyl deriv., which was heated with 2-chloroquinoline at 100.degree. for 1 h to give 7-benzyl-3-(2-quinolinyl)-3,7-diazabicyclo[3.3.1]nonane. I may be useful for the treatment of central nervous system diseases, disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neurodegeneration inflammation, pain, and drug withdrawal symptoms.

ACCESSION NUMBER: 2001:453062 CAPLUS  
DOCUMENT NUMBER: 135:61360  
TITLE: Preparation of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands.  
INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Nielsen, Simon Feldbaek; Ahning, Philip K.; Jorgensen, Tino Dyhring  
PATENT ASSIGNEE(S): Neurosearch A/S, Den.  
SOURCE: PCT Int. Appl., 34 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044243	A2	20010621	WO 2000-DK696	20001214
WO 2001044243	A3	20021031		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1274710	A2	20030115	EP 2000-983080	20001214
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
US 2003004153	A1	20030102	US 2002-130099	20020514
PRIORITY APPLN. INFO.:			DK 1999-1790	A 19991214
			WO 2000-DK696	W 20001214
OTHER SOURCE(S):	MARPAT 135:61360			
IT	286945-99-1P 286946-00-7P 286946-07-4P 345317-15-9P 345317-16-0P 345317-17-1P			

345317-18-2P 345317-19-3P 345317-20-6P

345317-21-7P 345317-22-8P 345317-23-9P

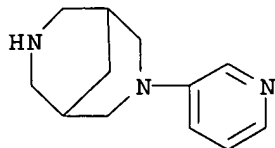
345317-24-0P 345317-26-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands)

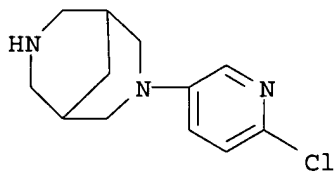
RN 286945-99-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)



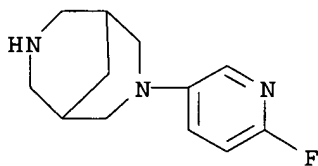
RN 286946-00-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



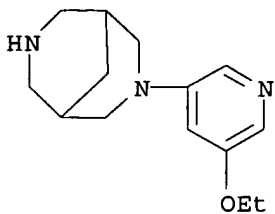
RN 286946-07-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



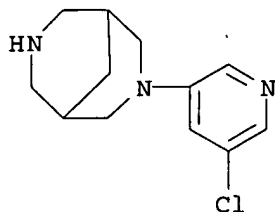
RN 345317-15-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



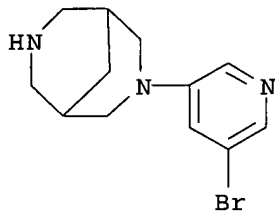
RN 345317-16-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



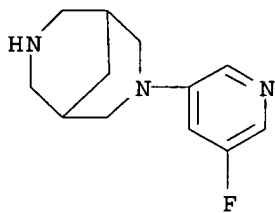
RN 345317-17-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-bromo-3-pyridinyl)- (9CI) (CA INDEX NAME)



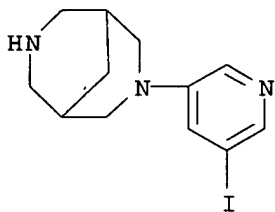
RN 345317-18-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)

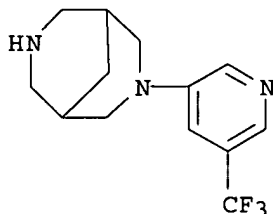


RN 345317-19-3 CAPLUS

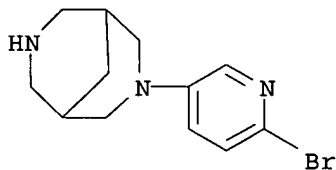
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)



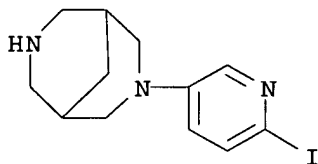
RN 345317-20-6 CAPLUS  
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[5-(trifluoromethyl)-3-pyridinyl]- (9CI)  
(CA INDEX NAME)



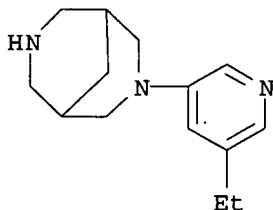
RN 345317-21-7 CAPLUS  
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-bromo-3-pyridinyl)- (9CI) (CA INDEX NAME)



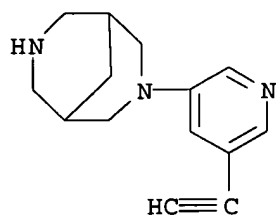
RN 345317-22-8 CAPLUS  
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-23-9 CAPLUS  
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

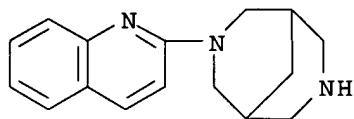


RN 345317-24-0 CAPLUS  
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethynyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

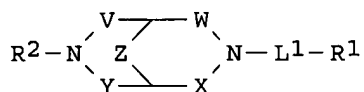


RN 345317-26-2 CAPLUS

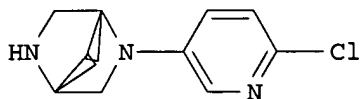
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-quinolinyl) - (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS  
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I



II

AB The title compds. (I) [wherein V and X = independently a bond or CH<sub>2</sub>; W and Y = independently a bond, CH<sub>2</sub>, or CH<sub>2</sub>CH<sub>2</sub>; Z = CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, or CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>; L<sub>1</sub> = a bond or (CH<sub>2</sub>)<sub>n</sub>; n = 1-5; R<sub>1</sub> = certain heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R<sub>2</sub> = H, alkoxycarbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH<sub>2</sub>] and their pharmaceutically acceptable salts were prepd. as cholinergic modulators for the treatment of pain and other conditions. For example, (-)-II.bul.Ts-OH was prepd. in a multi-step sequence involving N-protection of (1R,4R)-2-benzyl-2,5-diazabicyclo[2.2.1]heptane.bul.2HBr with CO(OBu-t)<sub>2</sub> (94%), debenzylation (93%), addn. of 2-chloro-5-iodopyridine (67%), and deprotection followed by salt formation (71%). (-)-II.bul.Ts-OH exhibited high affinity for the nicotinic acetylcholine receptor with K<sub>i</sub> of 0.01 nM and showed a significant antinociceptive effect at the minimally ED of 0.62 .mu.mol/kg in the mouse hot plate paradigm.

ACCESSION NUMBER: 2000:535147 CAPLUS  
DOCUMENT NUMBER: 133:135332  
TITLE: Preparation of diazabicyclic derivatives as nicotinic acetylcholine receptor ligands  
INVENTOR(S): Bunnelle, William H.; Cristina, Daniela Barlocco; Daanen, Jerome F.; Dart, Michael J.; Meyer, Michael D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy, Kevin B.; Toupence, Richard B.  
PATENT ASSIGNEE(S): Abbott Laboratories, USA  
SOURCE: PCT Int. Appl., 123 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044755	A1	20000803	WO 2000-US1620	20000125
W: AE, AL, AM, <del>AT</del> , AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1147112	A1	20011024	EP 2000-906998	20000125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000007664	A	20020507	BR 2000-7664	20000125
JP 2002535409	T2	20021022	JP 2000-596011	20000125



NO 2001003731 A 20010918 NO 2001-3731 20010730  
 BG 105836 A 20020329 BG 2001-105836 20010822  
 PRIORITY APPLN. INFO.: US 1999-239838 A 19990129  
 WO 2000-US1620 W 20000125

OTHER SOURCE(S): MARPAT 133:135332

IT **286945-99-1P**, 3-(3-Pyridinyl)-3,7-diazabicyclo[3.3.1]nonane

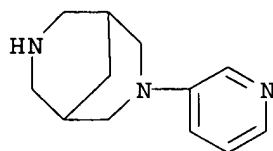
**286946-00-7P**, 3-(6-Chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine receptor ligands by addn. of haloheterocycles to protected diazabicycloalkanes followed by deprotection and optional substitution)

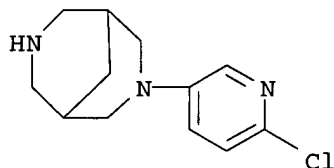
RN 286945-99-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286946-00-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



IT **286946-01-8P**, 3-(6-Chloro-5-methyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-02-9P**, 3-(5,6-Dichloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-03-0P**, 3-(6-Chloro-5-ethynyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-04-1P**, 3-(6-Chloro-5-cyano-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-05-2P**, 3-(5-Methoxy-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-06-3P**, 3-(6-Fluoro-5-methyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-07-4P**, 3-(6-Fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-08-5P**, 3-(5-Ethynyl-6-fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-09-6P**, 3-(5-Cyano-6-fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-10-9P**, 3-(5-Bromo-6-chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286947-18-0P**, 3-(3-Pyridinyl)-3,7-diazabicyclo[3.3.1]nonane bis(4-methylbenzenesulfonate) **286947-19-1P**, 3-(6-Chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane 4-methylbenzenesulfonate

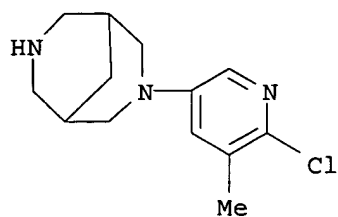
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine

receptor ligands by addn. of haloheterocycles to protected  
diazabicycloalkanes followed by deprotection and optional substitution)

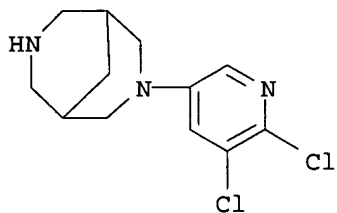
RN 286946-01-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-methyl-3-pyridinyl)- (9CI)  
(CA INDEX NAME)



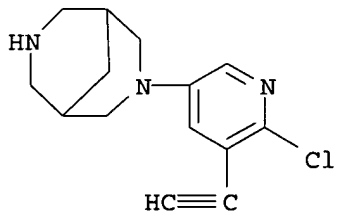
RN 286946-02-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5,6-dichloro-3-pyridinyl)- (9CI) (CA  
INDEX NAME)



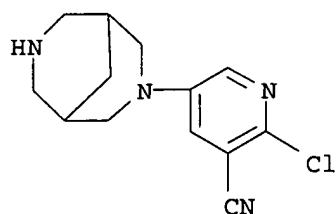
RN 286946-03-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-ethynyl-3-pyridinyl)- (9CI)  
(CA INDEX NAME)



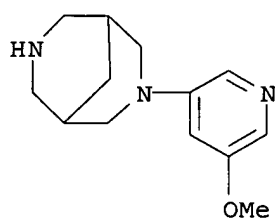
RN 286946-04-1 CAPLUS

CN 3-Pyridinecarbonitrile, 2-chloro-5-(3,7-diazabicyclo[3.3.1]non-3-yl)-  
(9CI) (CA INDEX NAME)



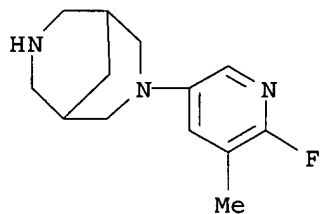
RN 286946-05-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



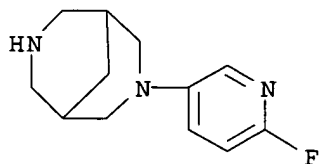
RN 286946-06-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-5-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



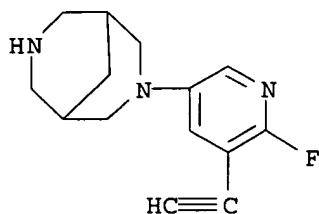
RN 286946-07-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)

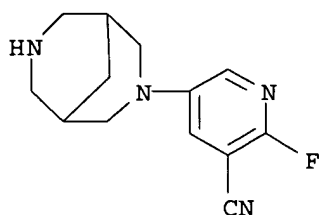


RN 286946-08-5 CAPLUS

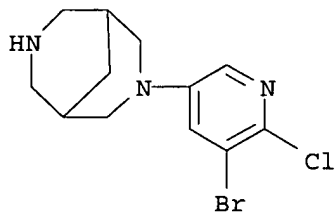
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethynyl-6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286946-09-6 CAPLUS  
 CN 3-Pyridinecarbonitrile, 5-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-fluoro-  
 (9CI) (CA INDEX NAME)



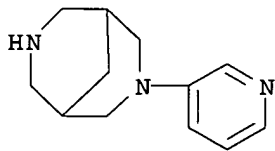
RN 286946-10-9 CAPLUS  
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-bromo-6-chloro-3-pyridinyl)- (9CI)  
 (CA INDEX NAME)



RN 286947-18-0 CAPLUS  
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

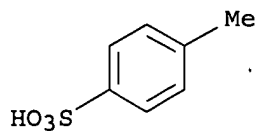
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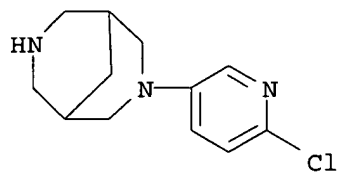
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CMF C7 H8 O3 S



RN 286947-19-1 CAPLUS  
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)-,  
mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

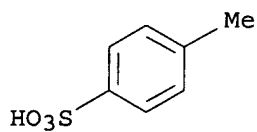
CM 1

CRN 286946-00-7  
CMF C12 H16 Cl N3



CM 2

CRN 104-15-4  
CMF C7 H8 O3 S



REFERENCE COUNT: 4. THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

05/14/2003

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LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

24.35

177.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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-3.26

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